

frac. valid SMILES

1.0
0.5

frac. unique SMILES

1.0
0.5

frac. SMILES in train

0.05
0.00
-0.05

frac. SMILES in PubChem

1
0

KLD

0.5
0.0

Frechet distance

25
0

frac. SMILES with azo

1
0

SA score

2.5
0.0

0.0 0.5 1.0 1.5 2.0
temperature

